L6 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2000 ACS ACCESSION NUMBER: 1999:487218 CAPLUS DOCUMENT NUMBER: 131:116106 TITLE: synthesis and antibacterial activity of tetracycline

INVENTOR(S): PATENT ASSIGNEE(S): SOURCE:

compds.

Levy, Stuart B., Nelson, Mark L.
Trustees of Tufts College, USA
PCT Int. Appl., 47 pp.
CODEN: PIXXD2
Patent
English
2

DOCUMENT TYPE:

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

KIND DATE APPLICATION NO. DATE PATENT NO. 937307 Al 19990729 WO 1999-US1393 19990122 W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, WO 9937307 DE.

DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP. KE, KG, KP, KR, K2, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN,

MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TH, TR. TT. UA. UG. US. UZ. VN. YU. ZW. AM, AZ, BY, KG, KZ, MD. RU.

TJ, TM
RW: GH, GM, KE, LS, MW, SD, S2, UG, ZW, AT, BE, CH, CY, DE, DK, ES. FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG,

CH, GA, GN, GW, ML, HR, NE, SN, TD, TG

AU 9924660 A1 19990809 AU 1999-24660 19990122

PRIORITY APPLN. INFO: US 1998-PV72262 19980123

WO 1999-US1393 19990122

OTHER SOURCE(S): MARPAT 131:116106

OTHER SOURCE(5): MARPAT 131:116106

AB Synthesis of substituted tetracycline compds. (I) (R1 = alkyl, alkenyl, alkynyl, alkoxy, alkylthio, alkylsulfinyl, alkylsulfonyl, alkylamino, arylalkyl, R2 = alkanoyl, arcyl, alkylarcyl, carbacyclic aryl, alkylsulfinyl, alkylsulfinyl, alkynyl, alkoxy, alkylthio, alkylsulfinyl, alky

and gram-pos. and gram-neg, tetracycline sensitive and tetracycline resistant

ANSWER 1 OF 2 CAPLUS COPYRIGHT 2000 ACS (Conti)

233586-01-1 CAPLUS 2-Naphthacenecarboxamide, 4-(d) ethvlamino)-9-[1,1-dimethvl-2-(1piperidinyl)ethyl]-1,4,4a,5,5a,6,1,12a-octahydro-3,10,12,12a-tetrahydroxy-6-methyl-1,11-dioxo-5-(1-oxopropoxy)-, (45,4ar,55,5ar,6r,12as)- (9CI)

(CA INDEX NAME)

Absolute stereochemistry.

cenecarboxamide, 5-(acetyloxy)-4-(dimethylamino)-9-(1,1-

dimethylethyl)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-6-methyl-1,11-dioxo-, (45,4aR,55,5aR,6R,12aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 1 OF 2 CAPLUS COPYRIGHT 2000 ACS (Continued) bacteria is presented. Thus, I (R1 = Me3C, R2 = EtCO, R3 = H) (II)

prepd. in two steps by acylation of doxycycline with propionic acid followed by alkylation with t-butanol. II showed and MIC of $6.25\,$

prepo. in two ways of the property of the prop

Absolute stereochemistry.

233586-00-0 CAPLUS

2-Naphthacenerarboxamide, -chloro-1,1-dimethylethyl)-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-6-methyl-1,11-dioxo-5-(1-oxopropoxy)-, (45,4aR,5S,5aR,6R,12aS)- (9CI) (CA INDEX

Absolute stereochemistry.

ANSWER 1 OF 2 CAPLUS COPYRIGHT 2000 ACS (Continued):

233586-14-6 CAPLUS
Benzeneacetic acid, (45,4aR,55,5aR,6R,12a5)-2-(aminocarbonyl)-4(dimethylamino)-9-(1,1-dimethylethyl)-1,4,4a,5,5a,6,11,12a-octahydro3,10,12,12a-tetrahydroxy-6-methyl-1,11-dioxo-5-naphthacenyl ester

(CA INDEX NAME)

RN 233586-23-7 CAPLUS
CN 2-Naphthacenecarboxamide, 5-(acetyloxy)-4-(dimethylamino)-9-[2-(dimethylamino)-1,1-dimethylethyl]-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tectrahydroxy-6-methyl-1,11-dioxo-,
(45,4a,5,5a,6a,6R,12aS)(9CI) (CA INDEX NAME)

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ANSWER 1 OF 2 CAPLUS COPYRIGHT 2000 ACS (Continued) 23356-24-8 CAPLUS 2-13586-24-8 CAPLUS 2-Naphthacenecarboxamide, 4-(dimethylamino)-9-[2-(dimethylamino)-1,1-2-Naphthacenecarboxamide, 4-(dimethylamino)-9-[2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylamino)-1,1-2-(dimethylami
dimethylethyl]-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-6-
methyl-1,11-dioxo-5-(1-oxopropoxy)-, (45,4aR,55,5aR,6R,12aS)- (9CI)
                  INDEX NAME)
                   233586-26-0 CAPLUS
Benzeneacetic acid, (4S,4aR,5S,5aR,6R,12aS)-2-{aminocarbonyl}-4-
(dimethylamino)-9-[2-(dimethylamino)-1,1-dimethylethyl]-
1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-6-methyl-1,11-
dioxo-5-naphthacenyl ester (9CI) (CA INDEX NAME)
                                                                                                                 ,
Bernardi; US 3901942 A 1975
Levy; US 5258372 A 1978
Levy; US 5064821 A 1991 CAPLUS
 L6 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2000 ACS ACCESSION NUMBER: 1999:487217 CAPLUS DOCUMENT NUMBER: 131:116105
 DOCUMENT NUMBER:
TITLE:
                                                                                                 131:116105
synthesis and antibacterial activity of
tetracycline-type compounds
Levy, Stuart B., Nelson, Mark L.
Trustees of Tufts College, USA
PCT Int. Appl., 56 pp.
CODEN: PIXXD2
  INVENTOR(S):
  PATENT ASSIGNEE(S):
SOURCE:
  DOCUMENT TYPE:
  FAMILY ACC. NUM. COUNT:
PATENT INFORMATION:
                                                             KIND DATE
                                                                                                                                                                         APPLICATION NO. DATE
                    PATENT NO.
                                               7306 Al 19990729 WO 1999-US1343 19990122
AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ,
                     WO 9937306
 DE.
                                                   DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS,
 JP.
                                                   KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK,
 MN.
                                                   MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL,
  TM.
                                                   TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ.
 RU.
                                     TJ, TM
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK,
  ES.
                                                    FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG,
CI,

OM, GA, GN, GW, ML, MR, NE, SN, TD, TG

AU 9923346

Al 19990809

AU 1999-23346

PRIORITY APPLM. INFO.:

US 1998-PV72262
19980123

OTHER SOURCE(S):

MARPAT 131:116105

AB Synthesis of substituted tetracycline-type compds.

alkenyl, alkynyl, alkoxy, alkylthio, alkylsulfinyl, alkylsulfonyl, alkylamino, arylalkyl; R2 = alkanoyl, aroyl, alkylaroyl, carbacyclic aryl, heteroarom., alkyl, alkenyl, alkynyl, alkoxy, alkylthio, alkylsulfinyl, alkylsulfinyl, alkylsulfinyl,
  CI.
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heteroarom, aanji, aanan, akylanino, akylanlinyl, alkylaulfonyl, alkylamino, arylalkyl; R3 H, alkyl, alkenyl, alkynyl, alkylylulfonyl, alkylamino, akylamino, alkylamino, alky

alkoxy, alkyithio, airyisuating, alloyidid arylalkyl, carbacyclic aryl, heteroarom., heteroalicyclic that exhibit significant antibacterial activity, including against both gram-pos. and gram-neg. bacteria is presented. Thus, I (RV = Me3C, R2 = EtCO, R3 = H) (II)

prepd. in two steps by acylation of doxycycline with propionic acid followed by alkylation with t-butanol. II showed an MIC of 6.25

.mu.g/mL against methicillin resistant 5. aureus.
IT 23386-00-0P RCT (Biological activity or effector, except adverse); RCT (Reactant)

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L6 ANSWER 2/OF 2 CAPLUS COPYRIGHT 2000 ACS (Continued)
SPN (Synthetic preparation), THU (Therapeutic use), BIOL (Biological study), PREP (Preparation), USES (Uses)
(synthesis and antibacterial activity of tetracycline-type compds.)
RN 23586-00-0 CAPLUS
Z-Naphthacenecatboxamide,
9-(24chloro-1,1-dimethylethyl)-4-(dimethylamino)-
1,4,4,5,5,a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-6-methyl-1,11-
dioxo-5-(1-oxopropoxy)-, (4S,4aR,5S,5aR,6R,12aS)- (9CI) (CA INDEX
   Absolute stereochemistry
                 233585-95-0P 233586-01-1P 233586-02-2P 233586-14-6P 233586-23-7P 233586-24-8P 233586-50-2 233586-51-1P 233586-55-5P 233586-56-6P 233586-51-1P 233586-62-4P 233586-57-7P 233586-62-4P 233586-67-4P 233586-67-4P 233586-68-0P 235586-69-1P 233586-68-0P 235586-69-1P 233586-68-0P
                 NAME
   Absolute stereochemistry.
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L6 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2000 ACS (Continued)
(5) Levy; US 5589470 A 1996 CAPLUS
(7) Trustees Of Tufts College; WO 9308806 A1 1993
CAPLUS

ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2000 ACS (Continued)

233586-01-1 CAPLUS
2-Naphthacenecarboxamide, 4-(dimethylamino)-9-[1,1-dimethyl-2-(1-

piperidinyl)ethyl]-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-6-methyl-1,11-dioxo-5-(1-охоргороху)-, (4S,4aR,5S,5aR,6R,12aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 233586-02-2 CAPLUS CN 2-Naphthacenecarboxamide, 5-(acetyloxy)-4-(dimethylamino)-9-(1/1-

dimethylethyl)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-6-methyl-1,11-dioxo-, (4S,4aR,5S,5aR,6R,12aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

1.6 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2000 ACS ntinued)

233586-24-8 CAPLUS 2-Naphthacenecarboxamide, 4-(dimethylamino)-9-[2-(dimethylamino)-1,1-

dimethylethyl]-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-6-methyl-1,11-dioxo-5-(1-охоргороху)-/(45,4aR,55,5aR,6R,12aS)-(9CI)

INDEX NAME)

Absolute stereochemistry.

23586-26-0 CAPLUS
Benzeneactic acid, (45/4sR,55,5aR,6R,12as)-2-(aminocarbonyl)-4(dimethylamino)-9-12-(dimethylamino)-1,1-dimethylathyl]1,4,4a,5,5a,6,11,12a-dctahydro-3,10,12,12a-tetrahydroxy-6-methyl-1,11dioxo-5-naphthacenyl ster (9CI) (CA INDEX NAME)

Absolute stereochemistry./

L6 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2000 ACS (Continued)

233586-14-6 CAPLUS
Benzeneacetic acid, (45,4aR,55,5aR,6R,12aS)-2-(aminocarbonyl)-4(disethylamino)-9-(1,1²dimethylethyl)-1,4,4a,5,5a,6,11,12a-octahydro3,10,12,12a-tetrahydroxy-6-methyl-1,11-dioxo-5-naphthacenyl ester

(9CI) (CA INDEX NAME)

Absolute stere

RN 233586-23-7 CAPLUS
CN 2-Naphthacenecarboxamide, 5-(acetyloxy)-4-(dimethylamino)-9-{2(dimethylamino)-1,1-dimethylethyl]-1,4,4a,5,5a,6,11,12a-octahydro3,10,12,12a-tetrahydroxy-6-methyl-1,11-dioxo-,
(45,4a,5,5a,6,6R,12a5)(9CI) (CA INDEX NAME)

ANSWER 2 OF 2 CAPLUS COPYRIGHT 2000 ACS (Continued)

RN 233586-50-0 CAPLUS
CN 2-Naphthacenecarboxamide,
N-(cyclopentylthio)-4-(dimethylamino)-9-(1,1-

dimethylethyl)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-6-methyl-1,11-dioxo-5-(1-oxopropoxy)-, (45,4aR,55,5aR,6R,12aS)- (9CI)

INDEX NAME)

Absolute stereochemistry.

233586-51-1 CAPLUS
2-Naphthacenecarboxamide, N-(cyclopentylthio)-4-(dimethylamino)1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-6-methyl-1,11dioxo-5-(1-oxopropoxy)-9-[2-(1-piperidinyl)ethyl)-,
(45,4aR,55,5aR,6R,12aS)- (9CI) (CA INDEX NAME)

L6 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2000 ACS

233586-55-5 CAPLUS
2-Naphthacenecarboxamide, 5-(acetyloxy)-4-(dimethylamino)-9-(1,1-

dimethylethyl)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-6-methyl-N-(methylthio)-1,11-dioxo-, (45,4aR,55,5aR,6R,12aS)- (9CI) INDEX NAME)

Absolute stereochemistry.

233586-56-6 CAPUS
2-Naphthacenecarboxamide, 4-(dimethylamino)-9-(1,1-dimethylethyl)-N(ethylthio)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxymethyl-1,11-dioxo-5-(1-oxopropoxy)-, (45,4aR,55,5aR,6R,12aS)- (9CI)

INDEX NAME)

Absolute stereochemistry.

(Continued) L6 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2000 ACS

233586-63-5 CAPLUS
2-Naphthacenecarboxamide, N-(cycloburylthio)-4-(dimethylamino)-9-(1,1-

dimethylethyl)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-6-methyl-1,11-dioxo-5-(1-oxopropoxy)f, (4S,4aR,5S,5aR,6R,12aS)-(9CI)

INDEX NAME)

Absolute stereochemistry.

233586-66-8 CAPLUS Benzeneacetic cid, (45,4aR,55,5aR,6R,12aS)-4-(dimethylamino)-9-(1,1-

dimethylethyl) -1, 4, 4a, 5, 5a, 6, 11, 12a-octahydro-3, 10, 12, 12a-tetrahydroxy-6-methyl-1, 11/dioxo-2-[[(phenylthio)amino]carbonyl]-5-naphthacenyl ester (SCI) (CA'INDEX NAME)

Absolute stereochemistry.

L6 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2000 ACS (Continued)

RN 233586-57-7 CAPLUS
CN Pentanoic acid, (45.4aR, 55,5aR, 6R, 12aS)-4-(dimethylamino)-9-(1,1-dimethylethyl)-1,4,4e,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-6-methyl-1,11-diöxo-2-[[(propylthio)amino]carbonyl]-5-naphthacenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

233586-62-4 CAPLUS 2-Naphthacenecarboxamide, 5-(acetyloxy)-4-(dimethylamino)-9-(1,1-

dimethylethyl)-1,4,4s,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-6-methyl-N-[(3-methylbutyl)thio]-1,11-dioxo-, (4S,4aR,5S,5aR,6R,12aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 2 OF 2 CAPLUS COPYRIGHT 2000 ACS

233586-68-0 CAPLUS

233300-08-U CAP MUS
2-Naphthacenecarboxamide, 5-(acetyloxy)-N-(cyclopentylthio)-4(dimethylamino)-9-[2-(dimethylamino)-1,1-dimethylethyll1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-6-methyl-1,11dioxo-, (4S,4aR,5S,5aR,6R,12aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

233586-69-1 CAPLUS
2-Naphthacenecarboxamide, N-(cyclopentylthio)-4-(dimethylamino)-9-[2-(dimethylamino)-1,1-dimethylethyl]-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-6-methyl-1,11-dioxo-5-(1-охоргороху)-,(4S,4aR,5S,5aR,6R,12aS)- (9CI) (CA INDEX NAME)

L6 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2000 ACS (Continued)

RN 233586-71-5 CAPLUS CN Benzeneacetic acid, (45,4aR,55,5aR,6R,12aS)-2-7

[[(cyclopentylthio)amino]carbonyl]-4-(dimethylamino)-9-[2-(dimethylamino)-

1,1-dimethylethyl]-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-6-methyl-1,11-dioxo-5-naphthacenyl enter (9CI) (CA INDEX NAME)

Absolute stereochemistry.

(1) Su; US 5834450 A 1998

=> d ibib ab hitstr

L13 ANSWER 1 OF 1 USPATFULL
ACCESSION NUMBER: 75:43716 USPATFULL
TITLE: Tetracycline derivatives substituted in the 7 position

INVENTOR(S):

and process for preparing the same Bernardi, Luigi, Milan, Italy Colonna, Vincenzo, Milan, Italy De Castiglione, Roberto, Milan, Italy Masi, Paolo, Milan, Italy Societa' Farmaceutici Italia S.p.A., Milan, Italy (non-U.S. corporation)

PATENT ASSIGNEE (S):

PATENT INFORMATION: APPLICATION INFO.:

NUMBER DATE

US 3901942 19750826
US 1973-397691 19730917 (5)

NUMBER DATE

PRIORITY INFORMATION:
DOCUMENT TYPE:
PRIMARY EXAMINER:
LEGAL REPRESENTATIVE:
NUMBER OF CLAIMS:
LEGAL REPRESENTATIVE:
LEGAL REPRESENTATIVE:
LUBBLE COUNT:
T25
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB Process for the preparation of tetracycline derivatives substituted in
the 7 position communication first observed.

the 7 position comprising first obtaining tetracycline derivatives substituted in the 7 and 9 positions, transforming the substituent

in the 7 position into the desired substituent, and then eliminating the

the substituent in the 9 position. Invention further comprises products obtained during the course of the above process.

IT \$3108-30-8P (prepn. of)
N \$5108-30-8 USPATFULL
CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-9-(1,1-dimethylethyl)-

1,4,4a,5,5a,6,11,12a-octahydro-3,5,10,12,12a-pentahydroxy-6-methyl-1,11-dioxo- (9C1) (CA INDEX NAME)

L13 ANSWER 1 OF 1 USPATFULL (Continued)

=> d ibib ab hitstr 1-3

L14 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1999:487218 CAPLUS
DOCUMENT NUMBER: 131:116106
TITLE: 5ynthesis and antibactetracycline synthesis and antibacterial activity of Compos. Levy, Stuart B.; Nelson, Mark L. Trustees of Tufts College, USA PCT Int. Appl., 47 pp. CODEN: PIXXD2 Patent INVENTOR (5): PATENT ASSIGNEE (5): SOURCE: DOCUMENT TYPE: LANGUAGE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION: PATENT NO. KIND DATE APPLICATION NO. DATE 7307 A1 19990729 W0 1999-US1393 19990122 AL, AH, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, WO 9937307 DB. DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP. KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN. MW. MX. NO. NZ. PL. PT. RO. RU. SD. SE. SG. SI. SK. SL. TJ. TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES. FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, HL, HR, NE, SN, TD, TG

AU 9924660 Al 19990809 AU 1999-24660 19990122

PRIORITY APPLN. INFO.: US 1998-PV72262 19980123

OTHER SOURCE(S): MARPAT 131:116106

AB Synthesis of substituted tetracycline compds. (I) (R1 = alkyl, alkenyl, alkoxy, alkylthio, alkylsulfinyl, alkylsulfonyl, alkylsulfonyl, alkylsulfonyl, alkylsulfonyl, alkylsulfonyl, alkylsulfonyl, alkylsulfinyl, alkylsulfonyl, alkyls significant antibacterial activity, including gram-pos. In gramineg bacteria, and gram-pos. and gram-nag. tetracycline sensitive and stracycline resistant L14 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2000 ACS (Co CN Cyclobutanecarboxy (4S, 4aR, 5S, 5aR, 6R, 12aS)

laR, 5S, 5aR, 6R, 12aS) -2 (ami (dimethylamino) -9-(1, 1-di 3, 10, 12, 12a-tetrahydroxy-., nocarbony1)-4-nethylethy1)-1,4,4a,5,5a,6,11,12a-octahydro-5-methy1-1,11-dioxo-5-naphthacenyl ester (9CI) (CA INDEX NAME) Absolute stereochemistry

233586-02-2 CAP\$US
2-Naphthacenecarboxamide, 5-(acetyloxy)-4-(dimethylamino)-9-(1,1dimethylethyl) -1, 4, 44, 5, 5a, 6, 11, 12a-octahydro-3, 10, 12, 12a-tetrahydroxy-6-methyl-1, 11-dioso-, (45, 4aR, 55, 5aR, 6R, 12a5) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L14 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2000 ACS (Continued) bacteria is presented. Thus, I (R1 = Me3C, R2 = EtCO, R3 = H) (II)

prepd. in two steps by acylation of doxycycline with propionic acid followed by alkylation with t-butanol. II showed and MIC of 6.25

.mu.g/ml against methicillin resistant S. aureus IT 233585-94-99 233385-95-09 233585-96-12 233586-02-29 233386-13-59 233586-14-69 233586-15-79 233586-16-89 233586-17-99 233586-18-09 233587-82-19

RL: BAC (Biological activity or effector, except adverse); SPN

RL BAC (Biological activity or affector, except adverse); SPN
(Synthetic
(Preparation); THU (Therapeutic use); BIOL (Biological study); PREP
(Preparation); USSS (Uses)
(synthesis and antibacterial activity of tetracycline compds.)
RN 233585-94-9 CAPUS
CN 2-Naphthacenecarboxamids, 4-(dimethylamino)-9-(1,1-dimethylethyl)-

1,4,4a,5,5a,6,11,12a-octahydro-3,5,10,12,12a-pentahydroxy-6-methyl-1,11-dioxo-, (45,4aR,55,45aR,6R,12a5)- (9CI) (CA INDEX NAME)

233585-95-0 CAPLUS 23336546-04 CAT203646, 4-(dimethylamino)-9-(1,1-dimethylethyl)1,4,4,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-6-methyl-1,11dixes-6-(1-oxopropoxy)-, (45,4aR,55,5aR,6R,12aS)- (9C1) (CA INDEX

Absolute stereochemistry.

L14 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2000 ACS (Continued)

233586-13-5 CAPLUS
2-Naphthacenecarboxamide, 5-(benzoyloxy)-4-(dimethylamino)-9-(1,1-

dimethylethyl)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-6-methyl-1,11-dioxo-, (4S,4aR,5S,5aR,6R,12aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

233586-14-6 CAPLUS
Benzeneacetic acid, (4S,4aR,5S,5aR,6R,12aS)-2-(aminocarbonyl)-4-(dimethylamino)-9-(1,1-dimethylethyl)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-6-methyl-1,11-dioxo-5-naphthacenyl ester

(CA INDEX NAME)

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L14 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2000 ACS
                                               (Continued)
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233586-15-7 CAPLUS
Carbamic acid, dimethyl-, (45,4aR,55,5aR,6R,12aS)-2-(aminocarbonyl)-4(dimethylamino)-9-(1,1-dimethylethyl)-1,4,4a,5,5a,6,11,12a-octahydro3,10,12,12a-tetrahydroxy-6-methyl-1,11-dioxo-5-naphthacenyl ester

(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 233586-16-8 CAPLUS
CN Cyclopentanecarboxylic acid,
(S, 48, 55, 58, 68, 128)-2- (aminocarbonyl)-4(dimethylamino)-9-(1,1-dimethylethyl)-1,4,4a,5,5g,6,11,12a-octahydro3,10,12,12a-tetrahydroxy-6-methyl-1,11-dioxo-5-paphthacenyl ester

Absolute stereochemistry.

ANSWER 1 OF 3 CAPLUS COPYRIGHT 2000 ACS (Continued) 3,10,12,12a-tetrahydroxy-6-methyl-1,11-dioxo-5-naphthacenyl ester (CA INDEX NAME)

Absolute stereochemistry

233887-82-1 CAPMS
2-Naphthacenecarboxamide, 4-(dimethylamino)-9-(1,1-dimethylethyl)-5(formyfoxy)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-6methyld 1,11-dioxo-, (43,4aR,55,5aR,6R,12aS)- (9CI) (CA INDEX NAME)

7
(1) Bernardi; US 3901942 A 1975
(2) Levy; US 5258372 A 1978
(4) Levy; US 506421 A 1991 CAPLUS
(5) Levy; US 5589470 A 1996 CAPLUS
(7) Trustees Of Tufts College; WO 9308806 A1 1993
CAPLUS
(2) CAPLUS

CAPLUS
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2000 ACS (Continued)

233586-17-9 CAPLUS

RN #23386-11-9 CATIOS
CN Cyclohexanecarboxylic acid,
(45, 48R, 55, 58R, 6R, 12a5) -2 (aminocarbonyl) -4 (dimethylamino) -9 (1,1-dimethylethyl) -1, 4, 4a, 5, 5a, 6, 11, 12a-octahydro 3, 10, 12, 12a-tetrahydroxy-6-methyl-1, 11-dioxo-5-naphthacenyl ester

(CA INDEX NAME)

Absolute stereochemistry.

233586-18-0 CAPLUS

RN 233586-18-U CAPLUS
CN Cycloheptanecarboxylic acid,
(45,4aR,5S,5aR,6R,12aS)-2-(aminocarbonyl)-4(dimethylamino)-9-(1,1~dimethylathyl)-1,4,4a,5,5a,6,11,12a-octahydro-

L14 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1999:487217 CAPLUS
DOCUMENT NUMBER: 131:116105
Synthesis and antibacterial activity of tetracycline-type compounds
Levy, Stuart B., Nelson, Mark L.
PATENT ASSIGNEE(S): Tcustees of Tufts College, USA
PCT Int. Appl., 56 pp.
CODEN: PIXXO2
DOCUMENT TYPE: Patent
LANGUAGE: PAMILY ACC. NUM. COUNT: 2
FAMILY ACC. NUM. COUNT: 2

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

	PATENT	NO.		KI	ND	DATE			A	PPLI	CATI	ON N	٥.	DATE		
	WO 9937	204			1	1999	0720				^^ "		•	1999		
	w:	AL,	AM,	ΑT,	ΑU,	ΑZ,	BA,	BB,	BG,	BR,	BY,	CA,	CH,	CN,	CU,	CZ,
DE,																
		DK.	EE.	ES.	FI.	GB,	GD.	GE.	GH.	GM.	HR.	HU.	ID.	IL.	IN.	IS.
JP.																
		KK	VC.	N.D	VD.	KZ,	10	LV	t D	1.0	1 T	T 11	11/	wn	MC	MV
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		MW,	ΜX,	NO,	NZ,	PL,	PT,	RO,	RU,	SD,	SE,	SG,	51,	SK,	SL,	TJ,
TM,																
		TR,	TT,	UA,	UG,	US,	UZ,	VN,	ΥU,	ZW,	AM,	AZ,	BY,	KG,	KZ,	MD,
RU,																
		TJ.	TM													
	pw.			KK	T.S	MW,	SD	57	110	7W	AT	84	CH	CV	DE	DΕ
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		FI,	FR,	GB,	GR,	ΙE,	IT,	LU,	MC,	NL,	PT,	SE,	BF,	вэ,	CF,	CG,
CI,																
		CM,	GA,	GN,	G₩,	ML,	MR,	NE.	SN,	TD,	TG					

AU 1999-23346 19990122 US 1998-PV72262 19980123 WO 1999-US1343 19990122 AU 9923346 PRIORITY APPLN. INFO.:

OTHER SOURCE(s): MARPAT 131:116105

AB Synthesis of substituted tetracycline-type compds. (I) (R1 = alkyl, alkenyl, alkynyl, alkylthio, alkylsulfinyl, alkylsulfonyl, alkylamino, arylalkylr R2 = alkanoyl, aroyl, alkylsulfonyl, carbacyclic

aryl,
heteroarom., alkyl, alkenyl, alkynyl, alkoxy, alkylthio,
alkylsulfinyl,
alkylsulfonyl, alkylamino, arylalkyl, R3 = H, alkyl, alkenyl, alkynyl,
alkoxy, alkylthio, alkylsulfinyl, alkylsulfonyl, alkylamino,

alkoxy, alkylthio, alkylsulfinyl, alkylsulfonyl, alkylsmino, arylalkyl, carbacyclic aryl, heteroarom., heteroalicyclic) that exhibit significant antibacterial activity, including against both gram-pos. and gram-neg. bacteria is presented. Thus, I (R1 - Me3C, R2 - EtCO, R3 - H) (II)

prepd. in two steps by acylation of doxycycline with propionic acid followed by alkylation with t-butanol. II showed an MIC of 6.25

.mu.g/mL against methicillin resistant S. aureus. IT 233586-94-9P 233585-95-0P 233585-95-1P 233586-02-2P 233586-13-5P 233586-14-6P

L14 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2000 ACS
233586-15-79 233586-16-8P 233586-17-99
233586-18-0P
RI: BRC (Biological activity or effector, except adverse); SPN
(Synthetic
preparation); THU (Therapeutic use); BIOL (Biological study); PREP
(Freparation); USES (Uses)
(synthesis and antibacterial activity of tetracycline-type compds.)
RN 233585-94-9 CAPLUS
CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-9-(1,1-dimethylethyl)-

1,4,4a,5,5a,6,11,12a-octahydro-3,5,10,12,12a-pentahydroxy-6-methyl-1,11-dioxo-, (4S,4aR,5S,5aR,6R,12aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

233585-95-0 CAPLUS
2-Naphthacenecatboxamide, 4-(dimethylamino)-9-(1,1-dimethylethyl)1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-6-methyl-1,11dioxo-5-(1-охоргороху)-, (4S,4aR,5S,5aR,6R,12aS)- (9CI) (CA INDEX

Absolute stereochemistry.

RN 233585-96-1 CAPLUS CN Cyclobutanecarboxylic acid, (45,4aR,55,5aR,6R,12aS)-2-(aminocarbonyl)-4-

L14 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2000 ACS (Continued)

233586-14-6 CAPLUS
Benzeneacetic acid, (4S,4aR,5S,5aR,6R,12aS)-2-(aminocarbonyl)-4(dimethylamino)-9-(1,1-dimethylathyl)-1,4,4a,5,5a,6,11,12a-octahydro3,10,12,12a-tetrahydroxy-6-methyl-1,11-dioxo-5-naphthacenyl ester (9CI)

(CA INDEX NAME)

Absolute stereochemistry.

233586-15-7 6 LUS

Carbamic acid, dimethyl-, (4S,4aR,5S,5aR,6R,12aS)-2-(aminocarbonyl)-4-(dimethylamind)-9-(1,1-dimethylethyl)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-yetrahydroxy-6-methyl-1,11-dioxo-5-naphthacenyl ester

(9CI) (CA INDEX NAME)

Absolute stereschemistry.

L14 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2000 ACS (Continued) (dimethylamino)-9-(1,1-dimethylathyl)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-6-methyl-1,11-dioxo-5-naphthacenyl ester (CA INDEX NAME)

Absolute stereochemistry.

RN 233586-02-2 CAPLUS CN 2-Naphthacenecarboxamide, 5-(acetyloxy)-4-(dimethylamino)-9-(1,1-dimethylethyl)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-6-methyl-1,11-dioxo-, (45,4aR,55,5aR,6R,12aS)- (9CI) (CA INDEX NAME)

233586-13-5 CAPLUS 2-Naphthacenecarboxamide, 5-(benzoyloxy)-4-(dimethylamino)-9-(1,1-

dimethylethyl)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-6-methyl-1,11-dioxo-, (45,4aR,55,5aR,6R,12aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L14 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2000 ACS (Continued)

233586-16-8 CAPLUS

CM Cyclopentanecarboxylic acid,
(45.4am,55,5am,6m,12a5)-2-(aminocarbonyl)-4(dimethylamino)-9-(1,1-dimethylethyl)-1,4,4a,5,5a,6,11,12a-octahydro3,10,12,12a-tetrahydroxy-6-methyl-1,11-dioxo-5-naphthacenyl ester

(CA INDEX NAME)

Absolute stereochemistry.

233586-17-9 CAPLUS

RN 233586-17-9 CAPLUS
CN Cyclohexanecarboxylic acid,
(45,4aR,5s,5aR,6R,12aS)-2-(aminocarbonyl)-4(dimethylamino)-9-(1,1-dimethylethyl)-1,4,4a,5,5a,6,11,12a-octahydro3,10,12,12a-tetrahydroxy-6-methyl-1,11-dioxo-5-naphthacenyl ester

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L14 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2000 ACS
                                                                                                                       (Continued)
RN 233586-18-0 CABLUS
CN Cycloheptanecacboxylic acid,
(45,4aR,55,5aR,6R,12aS)-2-(aminocarbonyl)-4-
(dimethylamin)-9-(1,1-dimethylethyl)-1,4,4a,5,5a,6,11,12a-octahydro-
3,10,12,12a-fetrahydroxy-6-methyl-1,11-dioxo-5-naphthacenyl ester
(9CI)
(CA INDEX NAME)
```

L14 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER:
1974:477746 CAPLUS
DOCUMENT NUMBER:
81:77746
TITLE:
INVENTOR(S):
Bernardi, Luigii Colonna, Vincenzoi De
Castiglione, Roberto, Mami, Paolo Societa Farmaceutici Italia Ger. Offen., 39 pp. CODEN: GMXXBX Patent German 1 PATENT ASSIGNEE(S): SOURCE:

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

	PATENT NO.	KIND	DATE	APPLICATIO	N NO.	DATE	
	DE 2346535	A1	19740411	DE 1973-23	46535	19730915	
	DE 2346535	B2	19800911				
	DE 2346535	C3					
	NL 7312648	A	19740320	NL 1973-12	648	19730913	
	NL 158172	В	19781016				
	CA 999855	A1	19761116	CA 1973-18		19730913	
	FR 2208885	A1	19740628	FR 1973-33		19730914	
	JP 49069653	A2	19740705	JP 1973-10	4458	19730914	
	JP 57041458	B4	19820903				
	ZA 7307317	Α	19740925	ZA 1973-73	17	19730914	
	AU 7360333	A1	19750320	AU 1973-60	333	19730914	
	BE 804913	A1	19740318	BE 1973-13	5695	19730917	
	AT 7307996	A	19750615	AT 1973-79	96	19730917	
	AT 328613	В	19760325				
	US 3901942	Α	19750826	US 1973-39	7691	19730917	
	GB 1413347	Α	19751112	GB 1973-43			
	HU 167850		19751225	HU 1973-SO		19730917	
	ES 418809		19760316	ES 1973-41		19730917	
	SU 574145	D	19770925	SU 1973-19		19730917	
PRIC	RITY APPLN. INFO.			IT 1972-29		19720918	
AB	Tetracycline de		/R = H. R1	A C MA NH	2 Ma2	NCH2	
	ONHCH2; R2		(K - 11, K1 -	e.y., ne, nn	2, nez	NCn2,	
	= H, Me; R3 = H,	UR) M	ere prend h	t the melective		1 m + 4 m m m m	
	tetracycline de	civ (p	the O-positi	on followed	e alky	racion of a	
	substitution in	-b- 7	cne s-posici	des l'estantes	na ere	ctrobutite	
R2 •	Suppritution in	Cite /~	bosition and	dealkylacion.	Thus	, I (K = KI	•
F42	R3 = H) was alky	.1	M. 30.00				~~
R1 -	NO - II) Was alky	Taced	WICH MEZCICH	in (Mezw) SPO	to gi	ve 1 (r = me.	3C1
111							
over	R2 = R3 = H) whi	.cn was	nitrated Wit	EN KNOS and HE	tuen	nydrogenate	1
Over		n - M-	ac ni - 1910	no no			
	PtO2 to give I	K - Me.	3C, RI = NH2,	R2 = R3 = H)	Rea	ction of this	5
with	product with HCH	io in ti	ue bresence o	or ha-c tollow	ed by	dealkylation	
WITH							
	F3CSO3H in PhOMe	gave :	(R = R2 = F	13 - H, R1 - M	2N).	About 20 I v	se re
	prepd.						
ΙT	53108-30-8P						
	RL: SPN (Synthet	ic pre	paration); PF	EP (Preparation	(מכ		
	(prepn. of)						
RN	53108-30-8 CAPL						
CN	2-Naphthacenecar	boxamic	ie, 4-(dimeth	ylamino)-9-(1,	1-dim	ethylethyl)-	

L14 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2000 ACS (Continued)

1,4,4a,5,5a,6,11,12a-octahydro-3,5,10,12,12a-pentahydroxy-6-methyl-1,11-dioxo- (9CI) (CA INDEX NAME)

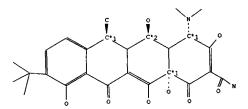
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L15 ANSWER 1 OF 1 BEILSTEIN COPYRIGHT 2000 BEILSTEIN CDES

Ring System Data:

Number of Rings (CNR): 4
Ring Systems (CNRS): 1
Diff. Ring Systems (CNDRS): 1
Ring Heteros (CNRH): 0
Acyclic Heteros (CNAH): 10

Beilstein Ring (BRIX)	1	(RF)	•		-1	BRIX Count
************	+			******	+	
18.4.12-0.0-5.	3 1	C18			i	1



Atom/Bond Notes: 1. CIP Descriptor: S 2. CIP Descriptor: R

Preparation:

L15 ANSWER 1 OF 1 BEILSTEIN COPYRIGHT 2000 BEILSTEIN CD&S (Continued) PRE

Reference(s):
1. Patent: Soc. Farm. Italia, DE 2346535 1974
Chem. Abstr., 81, 77746

CTUNCH Unchecked Data: NMR
Reference(s):
1. Patent: Soc. Farm. Italia, DE 2346535 1974
Chem. Abstr., 81, 77746
CTUNCH Unchecked Data: UV/VIS
Reference(s):
1. Patent: Soc. Farm. Italia, DE 2346535 1974
Chem. Abstr., 81, 77746

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	(FILE 'HOME' ENTERED AT 15:20:22 ON 03 JUN 2000)
L1 L2 L3 L4 L5	FILE 'REGISTRY' ENTERED AT 15:20:26 ON 03 JUN 2000 STRUCTURE UPLOADED 5 S L1 STRUCTURE UPLOADED 0 S L3 19 S L3 FULL
L6	FILE 'CAPLUS' ENTERED AT 15:24:06 ON 03 JUN 2000 2 S L5
ь7	FILE 'USPATFULL' ENTERED AT 15:25:14 ON 03 JUN 2000 0 S L5
L8	FILE 'MARPAT' ENTERED AT 15:25:26 ON 03 JUN 2000 0 S L5
L9 L10	FILE 'BEILSTEIN' ENTERED AT 15:25:53 ON 03 JUN 2000 0 S L3 FULL STRUCTURE UPLOADED
L11 L12	FILE 'REGISTRY' ENTERED AT 15:28:01 ON 03 JUN 2000 1 S L10 12 S L10 FULL
L13	FILE 'USPATFULL' ENTERED AT 15:28:40 ON 03 JUN 2000 1 S L12
L14	FILE 'CAPLUS' ENTERED AT 15:30:00 ON 03 JUN 2000 3 S L12
L15	FILE 'BEILSTEIN' ENTERED AT 15:33:26 ON 03 JUN 2000 1 S L10 FULL
	FILE 'REGISTRY' ENTERED AT 15:34:08 ON 03 JUN 2000